

ANOMALOUS BEHAVIOR OF THE COULOMB T-MATRIX

By William F. Ford [1963]

NASA Lewis Research Center, Cleveland, Ohio

ABSTRACT

(NASA TM X-50321)

Some apparent discrepancies in the definition or calculation of the Coulomb T-matrix are investigated in an approach that uses shielded wave functions. It is found that the screened Coulomb T-matrix behaves anomalously in the neighborhood of the energy shell and is in fact discontinuous in the limit of zero screening. A closed-form expression for the T-matrix, which has been derived previously, is shown to be essentially correct off the energy shell.

I. INTRODUCTION

In the usual application of the impulse approximation to a many-body scattering problem, it is common to introduce the two-body scattering matrix or T-matrix ($\underline{p}|T|\underline{k}$). The transition probability can then be expressed as an integral in which the T-matrix is folded into the product of the initial- and final-state momentum distributions.

Usually it is necessary to make further approximations, because experimental two-body scattering data give information about the T-matrix only on the energy shell $\underline{p}^2 = \underline{k}^2$. The most common approximation is to ignore off-the-energy-shell effects completely, putting $\underline{p}|T|\underline{k} \approx (\hat{k}\underline{p}|T|\underline{k})$. However, if the two-body scattering wave function is known exactly, the T-matrix can be directly calculated from the formula

$$(\underline{p}|T|\underline{k}) = \langle \Phi_{\underline{p}} | V | \Psi_{\underline{k}} \rangle \quad (1)$$

Here $\Psi_{\underline{k}}$ is the wave function for scattering by the potential V , and

$\Phi_{\underline{p}}$ is a final-state plane wave.

Available to NASA Offices and

NASA Centers Only

Since the Coulomb wave function is known exactly in closed form, it is natural to consider using the impulse approximation for atomic scattering problems. Such calculations have been made by Pradhan,¹ for instance, in the case of electron capture by protons, and by Akerib and Borowitz² in the case of electron scattering by atomic hydrogen.

Recently, however, there has been some doubt that the usual formal scattering theory, which leads to (1), is valid for a long range force such as the Coulomb force. Mapleton³ has evaluated the Coulomb wave operator

Ω CAPITAL GREEK OMEGA

$$\underline{\Omega}^{(+)} = i\epsilon(E + i\epsilon - K - V)^{-1/2}$$

by expanding it in Coulomb partial waves, and has shown that the function $\underline{\Omega}^{(+)}_{\frac{1}{2}k}$ differs from the usual Coulomb wave function by an energy-dependent factor. Previously Okubu and Feldman⁴ had studied the integral equation satisfied by $\underline{\Omega}^{(+)}$ in momentum space, obtaining a similar result. The T-matrix, which is related to the wave operator by $T = V\underline{\Omega}^{(+)}$, is thereby also in error.

Finally, one can show that the integral in (1), which has been evaluated for a Coulomb potential $V(r) = V_0/r$ by several authors,⁵ does not lead to the correct Coulomb scattering amplitude. For if a convergence factor $e^{-\lambda r}$ is used in (1), the result is

$$\langle \underline{p} | T | \underline{k} \rangle = \frac{V_0}{2\pi^2} \int d\eta e^{i\varphi\Delta} \lim_{\lambda \rightarrow 0} \frac{[\underline{p}^2 - (k + i\Delta)^2]^{1/2} i\eta}{[(\underline{p} - \underline{k})^2 + \lambda^2]^{1/2} (1 + i\eta)} \quad (2)$$

where

$$\eta = \frac{mV_0}{\hbar^2 k},$$

$$\begin{aligned} \varphi\Delta(\eta) &= e^{-\pi\eta/2} |\Gamma(1 + i\eta)|, \\ \varphi\Delta &= \arg \Gamma(1 + i\eta), \end{aligned} \quad (3)$$

and the principal values of the powers are to be taken. If we now set $p = k$ and take the limit $\lambda \rightarrow 0$, the scattering amplitude, which is $-4\pi\sqrt{m/\hbar}$ times the T-matrix, turns out to be

$$f_{\vec{k}}^{\sim}(\hat{r}) = f_{\vec{k}}^{\sim C}(\hat{r}) \left[\Gamma(1 - i\eta) e^{-i\eta \log(2k/\lambda)} \right], \quad (4)$$

where $f_{\vec{k}}^{\sim C}(\hat{r})$ is the usual expression⁶ for the Coulomb scattering amplitude:

$$f_{\vec{k}}^{\sim C}(\hat{r}) = - \frac{\eta}{2k \sin^2 \frac{1}{2}\theta} e^{2i\eta \log(\sin \frac{1}{2}\theta)}. \quad (5)$$

The squared modulus of the bracketed factor in Eq. (4) is $\eta/\sinh(\eta)$, similar to the extra factor found by Mapleton and by Okubu and Feldman. If the limit $\lambda \rightarrow 0$ is taken before setting $p = k$, an additional factor of

$$e^{\pm i\pi\eta/2} \quad (p \lessgtr k) \quad (6)$$

appears, so that (2) predicts a discontinuity at the energy shell as well as an incorrect scattering amplitude.

All of these difficulties seem to stem from the fact that the Coulomb potential distorts not only the scattered wave but also the incident plane wave. Thus for instance the integral equation

$$\psi_{\vec{k}}^{\sim} = \phi_{\vec{k}}^{\sim} + (E + i\epsilon - K)^{-1} \sqrt{m/\hbar} \psi_{\vec{k}}^{\sim}, \quad (7)$$

which is fundamental to formal scattering theory, is not strictly valid for Coulomb scattering. The same remark applies to the integral equation for the T-matrix, which is derived from (7). Recognizing this, Okubu and Feldman suggested either a renormalization or a cutoff procedure, designed

to make the T-matrix continuous at $p = k$ with the proper magnitude. Unfortunately, the functions so constructed do not then satisfy the integral equation, so that these procedures must be viewed with some caution.

One way to settle the question is to find the T-matrix for a screened Coulomb potential and study its behavior as the screening is turned off. In general this is a very difficult problem, although in principle it can be solved by an expansion of the T-matrix in spherical harmonics. If a discontinuity at the energy shell exists, however, the coefficient of each spherical harmonic will be affected; consequently, this point can be checked easily if one knows only the $l = 0$ component of the T-matrix.

There are two well-known potentials for which the $l = 0$ radial wave functions are known exactly, the cutoff Coulomb potential and the Hulthén potential.⁷ Both potentials can be made to resemble the ordinary Coulomb potential except at very large distances from the origin. In the following sections these radial wave functions are used to compute the $l = 0$ part of the T-matrix. In the limit of zero screening the results are identical, and show that there is indeed a discontinuity at the energy shell. They also indicate that Eq. (2) is essentially correct except when $\sqrt{2}/p = \sqrt{2}/k$.

II. EXPANSION IN SPHERICAL HARMONICS

We shall adopt delta-function normalization, so that for large r the wave function for a finite range potential is

$$\psi_{\vec{k}}(\vec{r}) \sim (2\pi)^{-3/2} \left[e^{i\vec{k} \cdot \vec{r}} + f_{\vec{k}}(\hat{r}) \frac{e^{ikr}}{r} \right], \quad (8)$$

with

$$\frac{f_{\vec{k}}(\hat{r})}{\sqrt{4\pi}} = - \frac{\sqrt{2m}}{\hbar^2} (\vec{k}\hat{r}|T|\vec{k}) \quad (9)$$

and

$$(\vec{p}|T|\vec{k}) = (2\pi)^{-3/2} \int e^{-i\vec{p}\cdot\vec{r}} V(r) \psi_{\vec{k}}(\vec{r}) d\vec{r}. \quad (10)$$

The expansion of $\psi_{\vec{k}}(\vec{r})$ in spherical harmonics may then be written in

the familiar form

$$\psi_{\vec{k}}(\vec{r}) = (2\pi)^{-3/2} \sum_{l=0}^{\infty} i^l (2l+1) P_l(\hat{k}\cdot\hat{r}) e^{i\delta_l} \frac{F_l(kr)}{kr}, \quad (11)$$

$$F_l(kr) \sim \sin(kr - \frac{1}{2}\pi l + \delta_l). \quad (12)$$

For the corresponding expansion of the T-matrix we write

$$(\vec{p}|T|\vec{k}) = - \frac{\sqrt{2m}}{4\pi\hbar^2} \sum_{l=0}^{\infty} (2l+1) P_l(\hat{p}\cdot\hat{k}) (\vec{p}|T_l|\vec{k}), \quad (13)$$

where

$$(\vec{p}|T_l|\vec{k}) = - \frac{\sqrt{2m}}{\hbar^2} \int_{-1}^1 (\vec{p}|T|\vec{k}) P_l(\underline{\mu}) d\underline{\mu} \quad (\underline{\mu} = \hat{p}\cdot\hat{k}) \quad (14)$$

$$= - \frac{2m}{\hbar^2 k} e^{i\delta_l} \int_0^{\infty} j_l(pr) V(r) F_l(kr) r dr. \quad (15)$$

(In Eq. (13) the factor $\sqrt{2m}/4\pi\hbar^2$ has been separated from $(\vec{p}|T_l|\vec{k})$ to simplify many of the equations in later sections.) From the asymptotic form of $\psi_{\vec{k}}(\vec{r})$ one can show that

$$(\vec{k}|T_l|\vec{k}) = \frac{e^{2i\delta_l} - 1}{2ik}, \quad (16)$$

and of course the integral in Eq. (15) must yield the same result.

For later reference we also give the usual expansion⁶ of the Coulomb wave function:

$$\psi_{\vec{k}}^{\text{C}}(\vec{r}) = (2\pi)^{-3/2} \sum_{l=0}^{\infty} i^l (2l+1) P_l(\hat{k} \cdot \hat{r}) e^{i g_l} \frac{F_l^{\text{C}}(kr)}{kr}, \quad (17)$$

$$F_l^{\text{C}}(kr) \sim \sin(kr - \frac{1}{2}\pi l - \eta \log 2kr + g_l), \quad (18)$$

$$g_l = \arg \Gamma(l+1+i\eta). \quad (19)$$

The charge parameter η is defined as in Eq. (3). The Coulomb radial wave functions $F_l^{\text{C}}(kr)$ may be expressed in terms of confluent hypergeometric functions:

$$\frac{F_l^{\text{C}}(kr)}{kr} = G_l(\eta)(2kr)^{-1/2} e^{i kr} {}_1F_1(l+1+i\eta; 2l+2; -2ikr), \quad (20)$$

$$G_l(\eta) = \frac{e^{-\pi\eta/2} |\Gamma(l+1+i\eta)|}{(2l+1)!} \quad (21)$$

It is customary⁸ to write

$$(k|F_l^{\text{C}}|k) = \frac{e^{2i g_l} - 1}{2ik} \quad (22)$$

for the pure Coulomb field, even though the series in Eq. 13 will not converge.

In the following sections we shall be concerned primarily with the calculation of F_0^{C} . For this purpose we introduce a related quantity $I(p)$, which is defined by

$$I(p) = \frac{2\pi}{\hbar^2 k} \int_0^{\infty} e^{i p r} V(r) F_0^{\text{C}}(kr) dr, \quad (23)$$

$$(\rho| \cancel{F_0}(k) = \frac{e^{-i\delta_0}}{2ip} [I(p) - I(p)^*]. \quad (24)$$

III. CUTOFF COULOMB POTENTIAL

Perhaps the simplest way to screen the Coulomb field is to cut it off at $r = R$, so that the potential is

$$V(r) = \begin{cases} \frac{V_0}{r} & r < R \\ 0 & r > R \end{cases} \quad (25)$$

Within this field the $l = 0$ wave function must be proportional to $\cancel{F_0}(kr)$, and outside it a sinusoid of unit amplitude; hence

$$\cancel{F_0}(kr) = \begin{cases} N \cancel{F_0}(kr) & r < R \\ \sin(kr + \delta_0) & r > R \end{cases}, \quad (26)$$

where N and δ_0 are to be determined. The correct procedure is to equate logarithmic derivatives at $r = R$, but to first order in $1/kR$ this is equivalent to matching amplitudes and phases. From Eq. (18) it follows that

$$N \sim 1, \quad \delta_0 \sim \delta_0 - \eta \log(2kR). \quad (27)$$

The next step is to calculate $I(p)$, which may be written

$$I(p) = 2\eta k N \cancel{F_0}(\eta) \int_0^R e^{i(k-p)r} \cancel{F_0}(1+i\eta; 2; -2ikr) dr. \quad (28)$$

When $p = k$, the integral can be performed directly, yielding

$$\begin{aligned} I(k) &= N \cancel{F_0}(\eta) \cancel{F_0}(i\eta; 1; -2ikr) \Big|_0^R \\ &= N \cancel{F_0}(\eta) \left[\frac{e^{-\pi\eta/2} (2kR)^{-i\eta}}{\Gamma(1-i\eta)} - 1 + \mathcal{O}\left(\frac{1}{kR}\right) \right] \\ &= e^{-i\delta_0} - N \cancel{F_0}(\eta). \end{aligned} \quad (29)$$

CAPITAL
SCRIPT
LETTER O

(In this derivation the asymptotic form of the $\frac{\Delta E}{1\sqrt{1}}$ function has been used, so that the result is apparently accurate only to order $1/kR$. It can be shown, however, that if logarithmic derivatives are equated to determine N and δ_0 , Eq. (29) is exact.) Thus we find that

$$(k|\frac{\Delta E}{1\sqrt{1}}|k) = \frac{e^{2i\delta_0} - 1}{2ik}, \quad (30)$$

as expected.

When $p \neq k$, $I(p)$ may be evaluated by using the integral representation

$$\frac{\Delta E}{1\sqrt{1}}(1 + i\eta; 2; -2ikr) = -\frac{1}{2\pi i} \int_C \left(\frac{t}{t-1}\right)^{i\eta} e^{-2ikrt} dt \quad (31)$$

and interchanging the order of integration:

$$I(p) = \frac{kN\frac{\Delta E}{1\sqrt{1}}(\eta)}{\pi i} \int_C \left(\frac{t}{t-1}\right)^{i\eta} \frac{1 - e^{iR(k-p-2kt)}}{k-p-2kt} dt. \quad (32)$$

For convenience the contour is taken to be that shown in Fig. 1, with principal values of $t^{i\eta}$ and $(t-1)^{-i\eta}$ to be used.

In the first term of Eq. (32) the contour is deformed and enlarged until it becomes a circle whose radius tends to infinity; here we must be careful to add a term canceling the contribution that comes from including the pole at $t' \equiv (k-p)/2k$. The integral around the large circle is then easily evaluated by expanding the integrand in powers of $1/t$. The second term in Eq. (32) is generally quite small and may be estimated by deforming the contour into straight lines in the lower half plane along $\text{Re}(t) = 0$ and $\text{Re}(t) = 1$, plus small circles about $t = 0$

and $t = 1$. All this leads to

$$I(p) = N C_{\infty}(\eta) \left[\left(\frac{t'}{t' - 1} \right)^{\frac{i\eta}{2}} - 1 \right] + O \left[\frac{1}{(p - k)R} \right]. \quad (33)$$

From Fig. 1 and the stipulation about principal values it is clear that

$$\arg \left(\frac{t'}{t' - 1} \right) = \begin{cases} 0 & p > k \\ -\pi & p < k \end{cases}; \quad (34)$$

hence our final result is

$$\begin{aligned} (p|T_{\infty}|k) = \frac{C_{\infty}(\eta)e^{\frac{i\delta_0}{2}}}{2ip} & \left\{ \left| \frac{p - k}{p + k} \right|^{\frac{i\eta}{2}} - \left| \frac{p + k}{p - k} \right|^{\frac{i\eta}{2}} \right\} \times \begin{cases} 1 & (p > k) \\ e^{\pi\eta} & (p < k) \end{cases} \\ & + O \left[\frac{1}{(p - k)R} \right]. \end{aligned} \quad (35)$$

The most remarkable feature of Eq. (35) is that, in the limit $R \rightarrow \infty$, it displays precisely the sort of discontinuity at the energy shell predicted by Eq. (2). Of course, the value of T_{∞} right on the energy shell is given correctly by Eq. (29) and cannot be obtained from Eq. (35). In fact, it is clear from Eq. (35) that these pronounced changes in magnitude take place within a narrow region about $p = k$, whose width is of the order of one over the range of the force. The significance of this result will be discussed in a later section.

IV. HULTHÉN POTENTIAL

To make sure that the results just obtained are not unique to the cutoff Coulomb potential, let us perform a similar calculation for a potential with exponential screening. We shall use the Hulthén potential

$$V(r) = \frac{V_0}{R} (e^{\sqrt{r/R}} - 1)^{-1} \rightarrow \begin{cases} \frac{V_0}{r} & r \ll R \\ \frac{V_0}{R} e^{-r/R} & r \gg R \end{cases} \quad (36)$$

for which the $l = 0$ radial wave function may be written in closed form:

$$F_0(kr) = N C_0(\eta) e^{i\sqrt{kr}} {}_2F_1(1 + i\alpha, 1 - i\beta; 2; z), \quad (37)$$

$$z = 1 - e^{-r/R}, \quad (38)$$

$$\alpha = kR \left(\sqrt{1 + \frac{2\eta}{kR}} - 1 \right), \quad \beta = \alpha + 2kR. \quad (39)$$

We assume R large enough that $|\eta/kR| \ll 1$; consequently α is real.

The normalization constant N and the phase shift are determined as usual by the asymptotic form of $F_0(kr)$. This may be obtained by expanding the hypergeometric function about $z = 1$, with the result that for $r \gg R$

$$F_0(kr) \sim N C_0(\eta) kR \left[\frac{\Gamma(i\beta - i\alpha)}{\Gamma(1 - i\alpha)\Gamma(1 + i\beta)} e^{i\sqrt{kr}} + \frac{\Gamma(i\alpha - i\beta)}{\Gamma(1 + i\alpha)\Gamma(1 - i\beta)} e^{-i\sqrt{kr}} \right] \quad (40)$$

Equation (40) may be written $F_0(kr) \sim \sin(kr + \delta_0)$ if we take

$$N = \frac{\beta}{2kRC_0(\eta)} \left| \frac{\Gamma(1 + i\alpha)\Gamma(i\beta)}{\Gamma(i\beta - i\alpha)} \right| \quad (41)$$

and

$$\delta_0 = \arg \frac{\Gamma(1 + i\alpha)\Gamma(i\beta - i\alpha)}{\Gamma(i\beta)}. \quad (42)$$

The case of interest is $R \rightarrow \infty$, so that $\alpha \rightarrow \eta$ and $\beta \rightarrow \infty$. We may therefore estimate the gamma functions by their asymptotic values, obtaining

$$\frac{\Gamma(i\beta - i\alpha)}{\Gamma(i\beta)} = \frac{\Gamma(2ikR)}{\Gamma(2ikR + i\alpha)} = (2ikR)^{-i\alpha} \left[1 + O\left(\frac{\eta}{kR}\right) \right]; \quad (43)$$

CAPITAL
SCRIPT
LETTER O

the normalization constant and the phase shift then take on the familiar values

$$N \sim 1, \quad \delta_0 \sim \varphi_0 - \frac{1}{2} \log(2kR). \quad (44)$$

It is also interesting to find the form of $F_0(kr)$ when $r \ll R$.

Using the relationship

$${}_2F_1(a, b; c; z) = {}_1F_1(a; c; bz) \left[1 + O\left(\frac{1}{b}\right) \right] \quad (45)$$

between ordinary and confluent hypergeometric functions, we may write

$$F_0(kr) = \cancel{F_0}(kr) \left[1 + O\left(\frac{r}{R}\right) + O\left(\frac{\eta}{kR}\right) \right], \quad (46)$$

a not unexpected result.

Let us turn now to the evaluation of $I(p)$, which in this case can be carried out exactly. After the variable of integration is changed to $z = 1 - \exp(-r/R)$, $I(p)$ becomes

$$I(p) = 2\eta k R N \cancel{C}(\eta) \int_0^1 (1-z)^{i\gamma} \cancel{F}_2(1+i\underline{\alpha}, 1-i\underline{\beta}; 2; z) dz, \quad (47)$$

where

$$\underline{\gamma} = (p - k)R. \quad (48)$$

This integral can be expressed⁹ in terms of a generalized hypergeometric function:

$$I(p) = \frac{2\eta k R N \cancel{C}(\eta)}{1+i\underline{\gamma}} \cancel{F}_{3/2}(1+i\underline{\alpha}, 1-i\underline{\beta}, 1; 2, 2+i\underline{\gamma}; 1). \quad (49)$$

We may simplify Eq. (49) considerably by invoking the series definitions

of the $\cancel{F}_{3/2}$ and \cancel{F}_2 functions and using the fact that $(1+a)_{\underline{n}} =$

$$(a)_{\underline{n+1}}/a:$$

CAPITAL
SCRIPT
LETTER O

$$\begin{aligned}
 I(p) &= \frac{2\eta k R N C \Lambda(\eta)}{1 + i\gamma} \sum_{n=0}^{\infty} \frac{(1 + i\alpha)_n (1 - i\beta)_n}{(2 + i\gamma)_n (n+1)!} \\
 &= \frac{2\eta k R N C \Lambda(\eta)}{\alpha\beta} \left[\frac{\Gamma(1 + i\alpha) \Gamma(1 - i\beta)}{\Gamma(2 + i\gamma)} - 1 \right] \\
 &= N C \Lambda(\eta) \left[\frac{\Gamma(1 + i\gamma) \Gamma(1 - i\alpha + i\beta + i\gamma)}{\Gamma(1 - i\alpha + i\gamma) \Gamma(1 + i\beta + i\gamma)} - 1 \right]. \quad (50)
 \end{aligned}$$

This expression is valid for all p . When $p = k$, $\gamma = 0$ and we get

$$I(k) = N C \Lambda(\eta) \left[\frac{\Gamma(1 - i\alpha + i\beta)}{\Gamma(1 - i\alpha) \Gamma(1 + i\beta)} - 1 \right] = e^{\frac{i\beta}{\alpha}} - N C \Lambda(\eta) \quad (51)$$

just as in Eq. (29); thus

$$(k|T|k) = \frac{e^{\frac{i\beta}{\alpha}} - 1}{2ik}. \quad (52)$$

When $p \neq k$, both β and γ are large compared to α . Again using the asymptotic form of the gamma function we obtain

$$I(p) = N C \Lambda(\eta) \left[(1 + i\gamma)^{\frac{i\eta}{\alpha}} (1 - i\alpha + i\beta + i\gamma)^{-\frac{i\eta}{\alpha}} - 1 \right] + \mathcal{O}\left[\frac{\eta}{(p-k)R}\right]. \quad (53)$$

Our final expression for $(p|T|k)$ is then

$$(p|T|k) = \frac{N C \Lambda(\eta) e^{\frac{i\beta}{\alpha}}}{2ip} \left[\left(\frac{p-k-i\lambda}{p+k-i\lambda} \right)^{\frac{i\eta}{\alpha}} - \left(\frac{p+k+i\lambda}{p-k+i\lambda} \right)^{\frac{i\eta}{\alpha}} \right] + \mathcal{O}\left[\frac{\eta}{(p-k)R}\right], \quad (54)$$

CAPITAL
SCRIPT
LETTER O

where $\lambda = 1/R$. This agrees perfectly with the result of the previous section in the region where both are valid, i.e., $|p - k| \gg 1/R$.

7. DISCUSSION

The foregoing analysis can of course be extended to values of η beyond $\eta = 0$, although results in closed form are possible only for the

cutoff Coulomb potential. It is well known¹⁰ that the phase shifts so obtained are given by

$$\delta_l \sim \eta \log(2kR), \quad (55)$$

provided that $l \ll kR$. When $l \gg kR$, the phase shifts fall rapidly to zero because of the angular momentum barrier; the intermediate region $l \approx kR$ is quite hard to handle.

Under the assumption, however, that R is so large as to make contributions from $l \lesssim kR$ generally negligible,¹⁰ comparison of Eqs. (11) and (17) reveals that

$$\psi_A(r) \cong e^{-i\eta \log 2kR} \psi_C(r), \quad r < R. \quad (56)$$

The equality does not hold for $r > R$ because $\psi_C(r)$ has logarithmic distortions not possessed by $\psi_A(r)$.

Let us now assume that $(p|T|k)$ is calculated as in the Introduction, but using Eq. (56), rather than just $\psi_C(r)$, as the approximation to $\psi_A(r)$. Quite obviously, the result is identical to Eq. (2) except that $e^{i\eta \log 2kR}$ is replaced by $e^{i\eta \log 2kR}$.

$$(p|T|k) = \frac{V_0}{2\pi^2} Q_0(\eta) e^{i\eta \log 2kR} \lim_{\lambda \rightarrow 0} \frac{[p^2 - (k + i\lambda)^2]^{1/2}}{[(p - k)^2 + \lambda^2]^{1/2}} \quad (2')$$

If we now expand Eq. (2') in Legendre polynomials according to Eq. (14), we find that

$$(p|T|k) = - \frac{V_0 Q_0(\eta) e^{i\eta \log 2kR}}{2p} \left[\frac{p^2 - (k + i\lambda)^2}{2pk} \right] A_l(x), \quad (57)$$

where

$$A_{\lambda}^{(x)} = \int_{-1}^1 P_{\lambda}(\mu) (x-\mu)^{-1-i\eta} d\mu \quad (58)$$

and

$$x = \frac{\sqrt{p^2} + \sqrt{k^2} + \sqrt{\lambda^2}}{2pk}. \quad (59)$$

We are primarily concerned with the coefficient A_0 , which is easily obtained:

$$A_0 = \frac{1}{i\eta} \left[(x-1)^{-1-i\eta} - (x+1)^{-1-i\eta} \right]. \quad (60)$$

Thus the $\lambda = 0$ component of Eq. (2) is given by

$$(p|T_0|k) = \frac{2\pi(\eta)e^{i\delta_0}}{2ip} \left[\left(\frac{p-k-i\lambda}{p+k-i\lambda} \right)^{i\eta} - \left(\frac{p+k+i\lambda}{p-k+i\lambda} \right)^{i\eta} \right]. \quad (61)$$

This agrees with the results of sec. III and IV when $\sqrt{p^2} \neq \sqrt{k^2}$, both in magnitude and phase (the limit $\lambda \rightarrow 0$ is understood). If the calculations of sec. III are repeated for higher values of λ , one again finds agreement with Eq. (57) for $\sqrt{p^2} \neq \sqrt{k^2}$. We are therefore led to the conclusion that the Coulomb T-matrix does possess a discontinuity at the energy shell, and that furthermore the T-matrix is correctly represented off the energy shell by Eq. (2), provided $e^{i\delta_0}$ is replaced by $e^{i\delta_0}$.

It is not difficult to see why Eq. (1) gives incorrect results on the energy shell when the approximation (56) is used. In the first place the Coulomb potential is a long-range potential, even though a convergence factor is used. Hence we may expect to get contributions from the asymptotic region of $\psi_{\lambda}^{(+)}(r)$, where the approximation is not valid. How-

ever, because the rapidly oscillating factors

$$\cancel{e^{-i(p \pm k)r}}$$

appear after the angular integration, contributions from the asymptotic region are negligible unless $|p - k| \sim 1/R$. This is precisely the condition found in sec. III and IV.

In summary, then, we have seen that the discontinuity in the T-matrix found by Okubu and Feldman and by Mapleton is quite real,¹¹ and that off the energy shell Eq. (2) is essentially correct. Thus, Eq. (1), which is a valid definition of the T-matrix for finite range forces, may also be used for the Coulomb force provided that shielding effects are taken into account when $\cancel{p^2} = \cancel{k^2}$.

ACKNOWLEDGMENTS

The author is indebted to Dr. V. A. Madsen and Prof. R. M. Thaler for several stimulating discussions of Coulomb scattering.

APPENDIX - COULOMB SCATTERING AMPLITUDE

We have deliberately ignored the problem of evaluating $(\underline{p}|T|\underline{k})$ on the energy shell, or the equivalent problem of finding the screened Coulomb scattering amplitude in the limit of zero screening. The customary way of doing this is to look at the coefficient of e^{ikr}/r in the asymptotic expansion of Eq. (56). We have seen, however, that Eq. (56) is valid only when $r < R$; it cannot be used when r is much larger than the range of the force. On the other hand, the experimental situation, in which measurements are made by a detector located well outside the range of the force, clearly corresponds to $r \gg R$.

One may argue that, as long as $kr \gg \eta$, it does not matter much whether $r < R$ or $r > R$; the asymptotic form changes very little. This is probably true, but it would be nice to have a direct verification such as we have presented here for the T-matrix off the energy shell. This involves performing the sum

$$\sum_l (2l+1) \frac{e^{2i\delta_l} - 1}{2ik} P_l(\cos \theta) \quad (A1)$$

where, for $kR \ll l$,

$$\delta_l = \sigma_l - \eta \log 2kR. \quad (A2)$$

(Incidentally, we note that $\sigma_l \sim \eta \log(l+1)$ for large l , so that the phase shifts δ_l approach zero as l approaches kR .)

At first we thought that Eq. (2) might have precisely the correct angular dependence on the energy shell, in spite of the fact that its magnitude is clearly wrong. However, upon evaluating A_l for $p^2 = k^2$, we find¹²

$$\begin{aligned}
 A_l &= \frac{1}{i\eta} \left(\frac{\lambda^2}{2k\lambda} \right)^{-i\eta} \left[\frac{\lambda^2}{2\lambda} \Gamma(-l, l+1; 1-i\eta; \frac{\lambda^2}{4k\lambda}) \right. \\
 &\quad \left. - \left(1 + \frac{4k\lambda^2}{\lambda^2} \right)^{-i\eta} e^{2i(\frac{\delta_l}{\lambda} - \frac{q_l}{\lambda})} \frac{\lambda^2}{2\lambda} \Gamma(-l, l+1; 1+i\eta; \frac{\lambda^2}{4k\lambda}) \right] \\
 &= -\frac{1}{i\eta} \left(\frac{\lambda^2}{2k\lambda} \right)^{-i\eta} \left[e^{2i(\frac{\delta_l}{\lambda} - \frac{q_l}{\lambda})} - 1 \right] + O\left(\frac{\eta}{k\lambda^2}\right) + O\left(\frac{l}{k\lambda^2}\right) \quad (A3)
 \end{aligned}$$

where as before $R = 1/\lambda$. Thus, the expansion of Eq. (2) on the energy shell (with $e^{i\frac{\delta_l}{\lambda}}$ replacing $e^{i\frac{q_l}{\lambda}}$) leads to

$$f_k(\hat{r}) = \Gamma(1+i\eta) \sum_{l=0}^L (2l+1) \frac{e^{2i(\frac{\delta_l}{\lambda} - \frac{q_l}{\lambda})} - 1}{2ik} P_l(\cos \theta) + \mathcal{R}, \quad (A4)$$

where L is very large but satisfies $L \ll kR$, $\frac{\delta_l}{\lambda}$ is given by Eq. (A2), terms of order η/kR have been ignored, and \mathcal{R} represents the rest of the series. It is evident that even apart from the factor $\Gamma(1+i\eta)$, the series in Eq. (A4) is different from that in (A1).

We could argue, as do Landau and Lifshitz,⁸ that the quantity

$$\sum_{l=0}^L (2l+1) P_l(\cos \theta)$$

approaches $2\delta(1 - \cos \theta)$ as $L \rightarrow \infty$ and so is only important when $\theta \leq \epsilon \sim 1/L$. In that case Eqs. (A1) and (A4) differ only by a factor of $\Gamma(1+i\eta) \exp(-2i\frac{q_l}{\lambda}) = \Gamma(1-i\eta)$ except at very small angles, provided that \mathcal{R} is negligible when $\theta > \epsilon$. (The factor $\Gamma(1-i\eta)$ has been noted previously; cf. Eq. (4).)

The above argument is not very satisfying, but since we have been unable to sum Eq. (A1), it will have to do. The prescription for

obtaining the T-matrix on the energy shell from Eq. (2) is then: (1) replace $e^{\frac{i\delta}{2}}$ by $e^{\frac{i\delta}{2}}$, (2) divide by $\Gamma(1 - i\eta)$. This causes Eq. (4) to become

$$f_{\tilde{k}}(\hat{r}) = f_{\tilde{k}}(\hat{r}) e^{-2i\eta \log 2kR}, \quad (A5)$$

the extra factor of $\exp(-i\eta \log 2kr)$ coming from step (1). Note that this expression for $f_{\tilde{k}}(\hat{r})$ may also be obtained from the asymptotic form of Eq. (56) if $r = R$. Assuming the correctness of Eq. (A5), we may then list the behavior of $\lim_{R \rightarrow \infty} |(p|T|k)|$ near the energy shell as follows:

$$\lim_{R \rightarrow \infty} |(p|T|k)| = \frac{1}{2\pi} \frac{1}{(p - k)^2} \times \begin{cases} \frac{1}{\sin \eta} & (p - k) \rightarrow 0^+ \\ 1 & p = k \\ e^{\frac{\pi\eta}{2}} \frac{1}{\sin \eta} & (p - k) \rightarrow 0^- \end{cases} \quad (A6)$$

REFERENCES

1. E. Pradhan, Phys. Rev. 125, 1250 (1957); E. Pradhan and D. N. Tripathy, Phys. Rev. 130, 2317 (1963).
2. R. Akerib and S. Barwitz, Phys. Rev. 122, 1277 (1961).
3. Robert A. Mapleton, J. Math. Phys. 2, 482 (1961); 3, 297 (1962).
4. Susumu Okubu and David Feldman, Phys. Rev. 117, 292 (1960).
5. A Nordisiek, Phys. Rev. 93, 785 (1954); E. Pradhan, Phys. Rev. 125, 1250 (1957).
6. L. I. Schiff, Quantum Mechanics (McGraw-Hill Book Company, Inc., New York, 1955), 2nd ed., pp. 114-120.
7. L. Hult  n, Ark. Mat. Astron. Fysik 28A, No. 5 (1942); 29B, No. 1 (1942).
8. L. D. Landau and E. M. Lifshitz, Quantum Mechanics, Non-Relativistic Theory (Addison-Wesley Publishing Company, Reading, Massachusetts, 1958), pp. 400-401, 419; Albert Messiah, Quantum Mechanics (North-Holland Publishing Company, Amsterdam, 1961), Vol. 1, p. 497.
9. Tables of Integral Transforms, Bateman Manuscript Project, edited by A. Erd  lyi (McGraw-Hill Book Company, Inc., New York, 1954), Vol. II, p. 399, eq. (5).
10. For a discussion see G. Breit, Rev. Modern Phys. 34, 766 (1963), sec. 4.
11. It should be pointed out, however, that the E-matrix obtained by these authors does not have the correct magnitude when $\frac{\sqrt{2}}{p} \neq \frac{\sqrt{2}}{k}$, although the discontinuity is correctly given.
12. See Ref. 3 for the method of performing the integral.

FIGURE LEGEND

Fig. 1 - Contour for evaluation of Eq. (32).

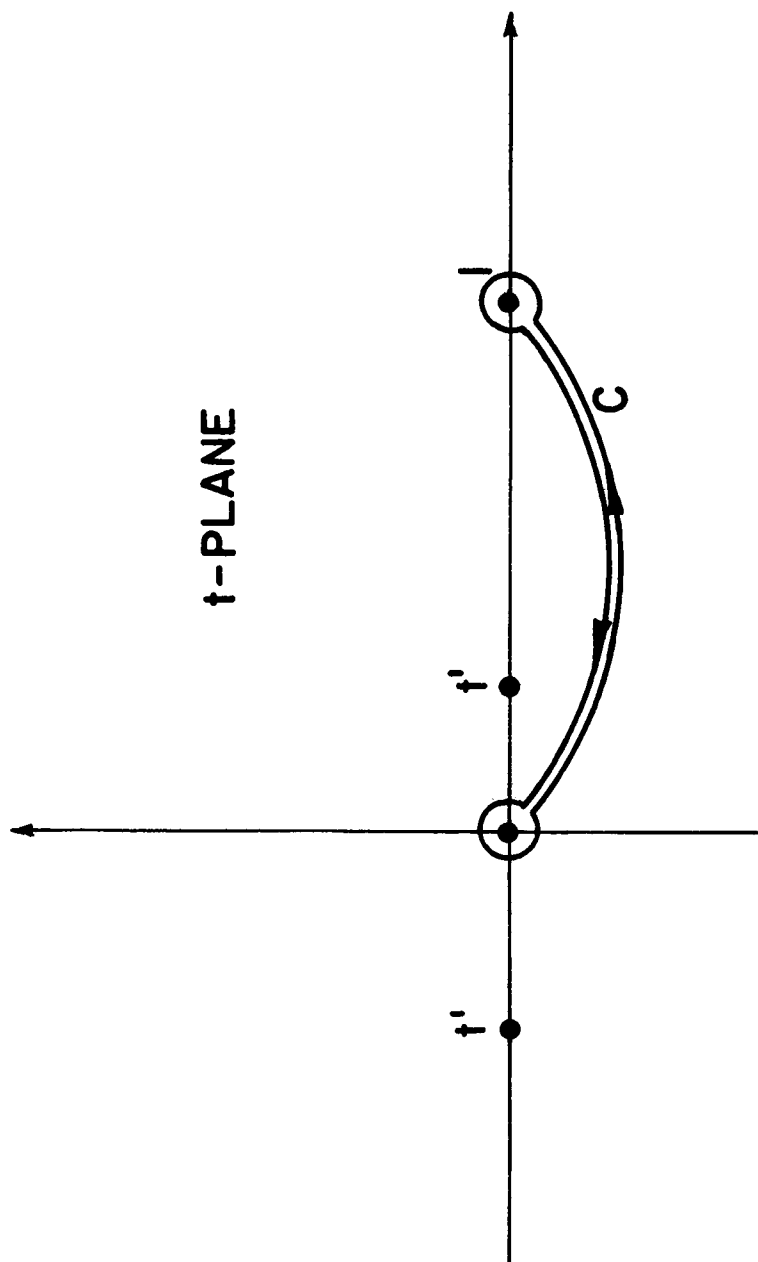


Fig. 1. - Contour for evaluation of Eq. (32).